

## THE ROTATIONAL SPECTRUM AND MOLECULAR PROPERTIES OF CHLORYL CHLORIDE, ClClO<sub>2</sub>

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ClClO<sub>2</sub> is slightly higher in energy than its structural isomer ClOOC<sub>l</sub>,<sup>a</sup> which has been implicated in polar ozone depletion processes. ClClOZ may be formed from other CL O<sub>2</sub> compounds on or in stratospheric ices.<sup>b</sup> Therefore, its millimeter and submillimeter spectrum has been studied in a flowing system as a product of the FClO<sub>2</sub> + HCl reaction. The pyramidal ClClOZ is an asymmetric prolate top,  $\kappa = -0.7598$  for <sup>35</sup>Cl<sup>35</sup>ClO<sub>2</sub>. It has *C<sub>s</sub>* symmetry with a strong dipole component along the c-axis and a smaller one along the a-axis. The highest quantum numbers accessed are larger than 50 and 30 for *J* and *K<sub>a</sub>*, respectively, permitting rotational and centrifugal distortion constants to be determined precisely. Splittings due to both Cl nuclei have been resolved, and a quadruple analysis will be presented. The molecular structure has been derived from isotopomers involving <sup>35</sup>Cl and <sup>37</sup>Cl. The results will be compared with those from an earlier matrix-isolation study,<sup>d</sup> from *ab initio* calculations,<sup>a</sup> and from data of related molecules.

<sup>a</sup>T. J. Lee, C. McMichael Rohlffing, and J. E. Rice, J. Chem. Phys., **97**, 6593, (1992)

<sup>b</sup>C. J. Pursell, J. Conyers, and C. Denisen, J. Phys. Chem., **100**, 15450, (1996)

<sup>c</sup>J. D. Graham, J. T. Roberts, L. D. Anderson, and V. H. Grassian, J. Phys. Chem. **100**, 19551, (1996)

<sup>d</sup>H. S. P. Müller and H. Winner, Inorg. Chem. **31**, 2527, (1992)

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